UNIVERSITI SAINS MALAYSIA

Peperiksaan Semester Kedua
Sidang Akademik 2002/2003

Februari/Mac 2003

KTE 211 – Kimia Takorganik II

Masa : 2 jam

Sila pastikan bahawa kertas peperiksaan ini mengandungi tujuh belas muka surat yang bercetak sebelum anda memulakan peperiksaan ini.

Kertas peperiksaan ini mengandungi dua bahagian iaitu, Bahagian A dan Bahagian B. **Jawab kedua-dua soalan di Bahagian A** dan **pilih dua lagi soalan daripada Bahagian B**. Jumlah soalan yang perlu dijawab ialah **EMPAT**.

Jika calon menjawab lebih daripada empat soalan hanya empat soalan pertama mengikut susunan dalam skrip jawapan akan diberi markah.

Jadual Karakter dilampirkan.

BAHAGIAN A

1. (a) Ramalkan spektrum IR dan Raman bagi sebatian piramid segiempat-sama, $Cr(CO)_4(CS)$ bagi getaran untuk CO dan CS.

(6 markah)

(b) Pemalar daya bagi C≡O ialah 1600 N m^{-1} dan bagi C≡Te ialah 400 N m^{-1} dapatkan nilai ν untuk getaran (C≡Te). J.A.R. C=12, O=16, Te=128

(6 markah)

(c) Berikan penjelasan bagi turutan nilai ν seperti berikut:

$\nu(C\text{-}H) > \nu(C{\equiv}O) > \nu(C{\equiv}Se) > \nu(Re{\equiv}Re) > \nu(Re\text{-}Re)$

(6 markah)

(d) Apakah yang maksudkan dengan istilah *satu sel unit*? Berikan enam parameter yang digunakan untuk menjelaskan satu sel unit dan nyatakan dua daripada jenis asas sel unit yang wujud.

(7 markah)

.../2-

2. (a) Takrifkan setiap istilah berikut dengan berdasarkan teori kumpulan:

(i) Operasi simetri

(ii) Paksi putaran wajar, C_n

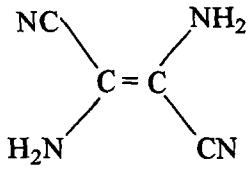
(iii) Kelas unsur simetri

(iv) Perwakilan terturunkan

(v) Perwakilan tak terturunkan

(15 markah)

(b) Dengan menggunakan kaedah matriks 3x3 (x, y, z) terbitkan set nilai karakter bagi setiap operasi simetri molecule berikut:



(10 markah)

BAHAGIAN B

3. Bagi setiap kaedah spektroskopi berikut:

(i) Inframerah (IR), (ii) Ultralembayung (UV) dan (iii) Resonans Magnetik Nuklear (NMR).

Tuliskan esei ringkas yang memperihalkan:

(a) Prinsip asas dan jenis tenaga yang diperlukan untuk kaedah masing-masing.

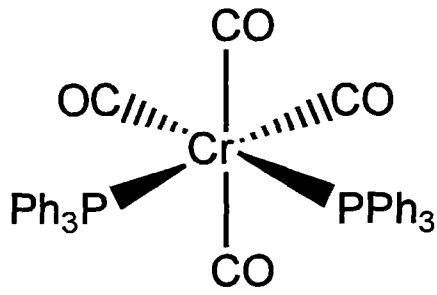
(8 markah)

(b) Keistimewaan dan kegunaan khusus masing-masing kaedah dalam mencirikan sesuatu sebatian takorganik.

(8 markah)

(c) Bincang dan lakarkan spektrum ramalan anda bagi setiap kaedah di atas untuk sebatian *cis*-$Cr(CO)_4(PPh_3)_2$ (struktur seperti berikut) dengan PPh_3 = *trifenilfosfina*, $P(C_6H_5)_3$.

(9 markah)



4. Gambarajah di bawah menunjukkan empat molekul A, B, C dan D.

(a) Tunjukkan kesemua operasi simetri yang terdapat pada setiap molekul tersebut dengan lakaran yang sesuai.

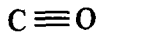
(9 markah)

(b) Berikan lakaran stereografik kumpulan titik bagi setiap molekul tersebut.

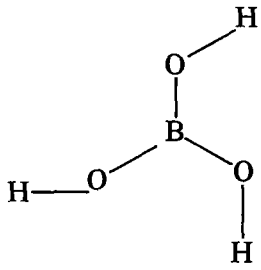
(8 markah)

(c) Berikan kumpulan titik bagi setiap molekul tersebut dan terangkan jawapan anda.

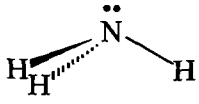
(8 markah)



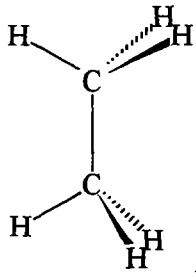
MOLEKUL A



MOLEKUL B



MOLEKUL C



MOLEKUL D

5. Berikan penjelasan terhadap kenyataan berikut:

(a) Spektrum NMR-^{13}C untuk sebatian $Fe(CO)_5$ menunjukkan hanya satu puncak pada suhu yang rendah.

(8 markah)

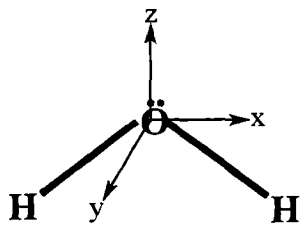
(b) Spektrum inframerah untuk ion sulfat, $[SO_4]^{2-}$ menunjukkan hanya satu jalur lebar pada ~1075 cm^{-1}. Tetapi bagi kompleks $[Co(NH_3)_5(SO_4)]Br$, kelihatan tiga jalur dalam spektrum inframerah.

(8 markah)

(c) Berbeza dengan kaedah spektroskopi fotoelektron-UV, kaedah spektroskopi fotoelektron sinaran-X dapat memberikan maklumat terperinci tentang tenaga pengikatan elektron pusat sesuatu sebatian.

(9 markah)

6. (a) Gambarajah di bawah menunjukkan molekul air yang dilakarkan berdasarkan paksi-paksi koordinat Cartes x, y dan z.



(i) Berikan kesemua unsur simetri yang wujud pada molekul tersebut.

(ii) Tentukan kumpulan titik bagi molekul tersebut.

(iii) Tentukan nilai karakter bagi setiap operasi dengan berdasarkan paksi koordinat Cartes yang diberikan bagi atom oksigen.

(17 markah)

(b) (i) Lakarkan molekul $Co(NH_3)_4Cl_2$ yang tergolong dalam kumpulan titik D_{4h} dan terangkan jawapan anda.

(ii) Dengan berpandukan teori kumpulan, bezakan antara isomer-isomer *cis* dan *trans* bagi molekul $PtBr_2Cl_2$.

(8 markah)

oooOooo

LAMPIRAN

Character Tables

THE NONAXIAL GROUPS

C_1	E
A	1

C_s	E	σ_h		
A'	1	1	x, y, R_z	x^2, y^2, z^2, xy
A''	1	−1	z, R_x, R_y	yz, xz

C_i	E	i		
A_g	1	1	R_x, R_y, R_z	$x^2, y^2, z^2, xy, xz, yz$
A_u	−1	−1	x, y, z	

THE AXIAL GROUPS

▸ *The C_n Groups*

C_2	E	C_2		
A	1	1	z, R_z	x^2, y^2, z^2, xy
B	1	−1	x, y, R_x, R_y	yz, xz

C_3	E	C_3	C_3^2	$\varepsilon = \exp(2\pi i/3)$	
A	1	1	1	z, R_z	$x^2 + y^2, z^2$
E	$\begin{Bmatrix}1\\1\end{Bmatrix}$	$\begin{matrix}\varepsilon\\ \varepsilon^*\end{matrix}$	$\begin{matrix}\varepsilon^*\\ \varepsilon\end{matrix}$	$(x, y), (R_x, R_y)$	$(x^2 - y^2, xy), (yz, xz)$

..., 8/

C_4	E	C_4	C_2	C_4^3		
A	1	1	1	1	z, R_z	$x^2 + y^2, z^2$
B	1	−1	1	−1		$x^2 - y^2, xy$
E	$\begin{Bmatrix}1 & i & -1 & -i\\ 1 & -i & -1 & i\end{Bmatrix}$				$(x, y), (R_x, R_y)$	(xz, yz)

C_5	E	C_5	C_5^2	C_5^3	C_5^4	$\varepsilon = \exp(2\pi i/5)$	
A	1	1	1	1	1	z, R_z	$x^2 + y^2, z^2$
E_1	$\begin{Bmatrix}1 & \varepsilon & \varepsilon^2 & \varepsilon^{2*} & \varepsilon^*\\ 1 & \varepsilon^* & \varepsilon^{2*} & \varepsilon^2 & \varepsilon\end{Bmatrix}$					$(x, y), (R_x, R_y)$	(yz, xz)
E_2	$\begin{Bmatrix}1 & \varepsilon^2 & \varepsilon^* & \varepsilon & \varepsilon^{2*}\\ 1 & \varepsilon^{2*} & \varepsilon & \varepsilon^* & \varepsilon^2\end{Bmatrix}$						$(x^2 - y^2, xy)$

C_6	E	C_6	C_3	C_2	C_3^2	C_6^5	$\varepsilon = \exp(2\pi i/6)$	
A	1	1	1	1	1	1	z, R_z	$x^2 + y^2, z^2$
B	1	−1	1	−1	1	−1		
E_1	$\begin{Bmatrix}1 & \varepsilon & -\varepsilon^* & -1 & -\varepsilon & \varepsilon^*\\ 1 & \varepsilon^* & -\varepsilon & -1 & -\varepsilon^* & \varepsilon\end{Bmatrix}$						$(x, y), (R_x, R_y)$	(xz, yz)
E_2	$\begin{Bmatrix}1 & -\varepsilon^* & -\varepsilon & 1 & -\varepsilon^* & -\varepsilon\\ 1 & -\varepsilon & -\varepsilon^* & 1 & -\varepsilon & -\varepsilon^*\end{Bmatrix}$							$(x^2 - y^2, xy)$

C_7	E	C_7	C_7^2	C_7^3	C_7^4	C_7^5	C_7^6	$\varepsilon = \exp(2\pi i/7)$	
A	1	1	1	1	1	1	1	z, R_z	$x^2 + y^2, z^2$
E_1	$\begin{Bmatrix}1 & \varepsilon & \varepsilon^2 & \varepsilon^3 & \varepsilon^{3*} & \varepsilon^{2*} & \varepsilon^*\\ 1 & \varepsilon^* & \varepsilon^{2*} & \varepsilon^{3*} & \varepsilon^3 & \varepsilon^2 & \varepsilon\end{Bmatrix}$							$(x, y), (R_x, R_y)$	(xz, yz)
E_2	$\begin{Bmatrix}1 & \varepsilon^2 & \varepsilon^{3*} & \varepsilon^* & \varepsilon & \varepsilon^3 & \varepsilon^{2*}\\ 1 & \varepsilon^{2*} & \varepsilon^3 & \varepsilon & \varepsilon^* & \varepsilon^{3*} & \varepsilon^2\end{Bmatrix}$								$(x^2 - y^2, xy)$
E_3	$\begin{Bmatrix}1 & \varepsilon^3 & \varepsilon^* & \varepsilon^2 & \varepsilon^{2*} & \varepsilon & \varepsilon^{3*}\\ 1 & \varepsilon^{3*} & \varepsilon & \varepsilon^{2*} & \varepsilon^2 & \varepsilon^* & \varepsilon^3\end{Bmatrix}$								

C_8	E	C_8	C_4	C_2	C_4^3	C_8^3	C_8^5	C_8^7	$\varepsilon = \exp(2\pi i/8)$	
A	1	1	1	1	1	1	1	1	z, R_z	$x^2 + y^2, z^2$
B	1	−1	1	1	1	−1	−1	−1		
E_1	$\begin{Bmatrix}1 & \varepsilon & i & -1 & -i & -\varepsilon^* & -\varepsilon & \varepsilon^*\\ 1 & \varepsilon^* & -i & -1 & i & -\varepsilon & -\varepsilon^* & \varepsilon\end{Bmatrix}$								$(x, y), (R_x, R_y)$	(xz, yz)
E_2	$\begin{Bmatrix}1 & i & -1 & 1 & -1 & -i & i & -i\\ 1 & -i & -1 & 1 & -1 & i & -i & i\end{Bmatrix}$									$(x^2 - y^2, xy)$
E_3	$\begin{Bmatrix}1 & -\varepsilon & i & -1 & -i & \varepsilon^* & \varepsilon & -\varepsilon^*\\ 1 & -\varepsilon^* & -i & -1 & i & \varepsilon & \varepsilon^* & -\varepsilon\end{Bmatrix}$									

▸ *The S_n Groups*

S_4	E	S_4	C_2	S_4^3		
A	1	1	1	1	R_z	$x^2 + y^2, z^2$
B	1	−1	1	−1	z	$x^2 - y^2, xy$
E	1	i	−1	$-i$	$(x, y), (R_x, R_y)$	(xz, yz)
	1	$-i$	−1	i		

S_6	E	C_3	C_3^2	i	S_6^5	S_6	$\varepsilon = \exp(2\pi i/3)$	
A_g	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
E_g	1	ε	ε^*	1	ε	ε^*	(R_x, R_y)	$(x^2 - y^2, xy)$, (xy, yz)
	1	ε^*	ε	1	ε^*	ε		
A_u	1	1	1	−1	−1	−1	z	
E_u	1	ε	ε^*	−1	$-\varepsilon$	$-\varepsilon^*$	(x, y)	
	1	ε^*	ε	−1	$-\varepsilon^*$	$-\varepsilon$		

S_8	E	S_8	C_4	S_8^3	C_2	S_8^5	C_4^3	S_8^7	$\varepsilon = \exp(2\pi i/8)$	
A	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
B	1	−1	1	−1	1	−1	1	−1	z	
E_1	1	ε	i	$-\varepsilon^*$	−1	$-\varepsilon$	$-i$	ε^*	(x, y), (R_x, R_y)	
	1	ε^*	$-i$	$-\varepsilon$	−1	$-\varepsilon^*$	i	ε		
E_2	1	i	−1	$-i$	1	i	−1	$-i$		$(x^2 - y^2, xy)$
	1	$-i$	−1	i	1	$-i$	−1	i		
E_3	1	$-\varepsilon^*$	$-i$	ε	−1	ε^*	i	$-\varepsilon$		(xz, yz)
	1	$-\varepsilon$	i	ε^*	−1	ε	$-i$	$-\varepsilon^*$		

▸ *The C_{nv} Groups*

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma'_v(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	−1	−1	R_z	xy
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	−1	R_z	
E	2	−1	0	$(x, y), (R_x, R_y)$	$(x^2 - y^2, xy), (xz, yz)$

../ 10-

C-4 APPENDIX C

C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$		
A_1	1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	−1	−1	R_z	
B_1	1	−1	1	1	−1		$x^2 - y^2$
B_2	1	−1	1	−1	1		xy
E	2	0	−2	0	0	$(x, y), (R_x, R_y)$	(xz, yz)

C_{5v}	E	$2C_5$	$2C_5^2$	$5\sigma_v$		
A_1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	−1	R_z	
E_1	2	2 cos 72°	2 cos 144°	0	$(x, y), (R_x, R_y)$	(xz, yz)
E_2	2	2 cos 144°	2 cos 72°	0		$(x^2 - y^2, xy)$

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$		
A_1	1	1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	1	−1	−1	R_z	
B_1	1	−1	1	−1	1	−1		
B_2	1	−1	1	−1	−1	1		
E_1	2	1	−1	−2	0	0	$(x, y), (R_x, R_y)$	(xz, yz)
E_2	2	−1	−1	2	0	0		$(x^2 - y^2, xy)$

► *The C_{nh} Groups*

C_{2h}	E	C_2	i	σ_h		
A_g	1	1	1	1	R_z	x^2, y^2, z^2, xy
B_g	1	−1	1	−1	R_x, R_y	xz, yz
A_u	1	1	−1	−1	z	
B_u	1	−1	−1	1	x, y	

C_{3h}	E	C_3	C_3^2	σ_h	S_3	S_3^5	$\varepsilon = \exp(2\pi i/3)$	
A'	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
E'	1	ε	ε^*	1	ε	ε^*	(x, y)	$(x^2 - y^2, xy)$
	1	ε^*	ε	1	ε^*	ε		
A''	1	1	1	−1	−1	−1	z	
E''	1	ε	ε^*	−1	$-\varepsilon$	$-\varepsilon^*$	(R_x, R_y)	(xz, yz)
	1	ε^*	ε	−1	$-\varepsilon^*$	$-\varepsilon$		

THE DIHEDRAL GROUPS

▸ *The* D_n *Groups*

D_2	E	$C_2(z)$	$C_2(y)$	$C_2(x)$		
A	1	1	1	1		x^2, y^2, z^2
B_1	1	1	−1	−1	z, R_z	xy
B_2	1	−1	1	−1	y, R_y	xz
B_3	1	−1	−1	1	x, R_x	yz

D_3	E	$2C_3$	$3C_2$	(x axis is coincident with C_2)	
A_1	1	1	1		$x^2 + y^2, z^2$
A_2	1	1	−1	z, R_z	
E	2	−1	0	$(x, y), (R_x, R_y)$	$(x^2 - y^2, xy), (xz, yz)$

D_4	E	$2C_4$	$C_2(=C_4^2)$	$2C_2'$	$2C_2''$	(x axis coincident with C_2')	
A_1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2	1	1	1	−1	−1	z, R_z	
B_1	1	−1	1	1	−1		$x^2 - y^2$
B_2	1	−1	1	−1	1		xy
E	2	0	−2	0	0	$(x, y), (R_x, R_y)$	(xz, yz)

D_5	E	$2C_5$	$2C_5^2$	$5C_2$	(x axis coincident with C_2)	
A_1	1	1	1	1		$x^2 + y^2, z^2$
A_2	1	1	1	−1	z, R_z	
E_1	2	2 cos 72°	2 cos 144°	0	$(x, y), (R_x, R_y)$	(xz, yz)
E_2	2	2 cos 144°	2 cos 72°	0		$(x^2 - y^2, xy)$

D_6	E	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$	(x axis coincident with C_2')	
A_1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2	1	1	1	1	−1	−1	z, R_z	
B_1	1	−1	1	−1	1	−1		
B_2	1	−1	1	−1	−1	1		
E_1	2	1	−1	−2	0	0	$(x, y), (R_x, R_y)$	(xz, yz)
E_2	2	−1	−1	2	0	0		$(x^2 - y^2, xy)$

C_{4h}	E	C_4	C_2	C_4^3	i	S_4^3	σ_h	S_4		
A_g	1	1	1	1	1	1	1	1	R_z	$x^2+y^2,\ z^2$
B_g	1	−1	1	−1	1	−1	1	−1		$x^2-y^2,\ xy$
E_g	1	i	−1	$-i$	1	i	−1	$-i$	(R_x, R_y)	(xz, yz)
	1	$-i$	−1	i	1	$-i$	−1	i		
A_u	1	1	1	1	−1	−1	−1	−1	z	
B_u	1	−1	1	−1	−1	1	−1	1		
E_u	1	i	−1	$-i$	−1	$-i$	1	i	(x, y)	
	1	$-i$	−1	i	−1	i	1	$-i$		

C_{5h}	E	C_5	C_5^2	C_5^3	C_5^4	σ_h	S_5	S_5^7	S_5^3	S_5^9	$\varepsilon = \exp(2\pi i/5)$	
A'	1	1	1	1	1	1	1	1	1	1	R_z	$x^2+y^2,\ z^2$
E_1'	1	ε	ε^2	ε^{2*}	ε^*	1	ε	ε^2	ε^{2*}	ε^*	(x, y)	
	1	ε^*	ε^{2*}	ε^2	ε	1	ε^*	ε^{2*}	ε^2	ε		
E_2'	1	ε^2	ε^*	ε	ε^{2*}	1	ε^2	ε^*	ε	ε^{2*}		(x^2-y^2, xy)
	1	ε^{2*}	ε	ε^*	ε^2	1	ε^{2*}	ε	ε^*	ε^2		
A''	1	1	1	1	1	−1	−1	−1	−1	−1	z	
E_1''	1	ε	ε^2	ε^{2*}	ε^*	−1	$-\varepsilon$	$-\varepsilon^2$	$-\varepsilon^{2*}$	$-\varepsilon^*$	(R_x, R_y)	(xz, yz)
	1	ε^*	ε^{2*}	ε^2	ε	−1	$-\varepsilon^*$	$-\varepsilon^{2*}$	$-\varepsilon^2$	$-\varepsilon$		
E_2''	1	ε^2	ε^*	ε	ε^{2*}	−1	$-\varepsilon^2$	$-\varepsilon^*$	$-\varepsilon$	$-\varepsilon^{2*}$		
	1	ε^{2*}	ε	ε^*	ε^2	−1	$-\varepsilon^{2*}$	$-\varepsilon$	$-\varepsilon^*$	$-\varepsilon^2$		

C_{6h}	E	C_6	C_3	C_2	C_3^2	C_6^5	i	S_3^5	S_6^5	σ_h	S_6	S_3	$\varepsilon = \exp(2\pi i/6)$	
A_g	1	1	1	1	1	1	1	1	1	1	1	1	R_z	$x^2+y^2,\ z^2$
B_g	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1		
E_{1g}	1	ε	$-\varepsilon^*$	−1	$-\varepsilon$	ε^*	1	ε	$-\varepsilon^*$	−1	$-\varepsilon$	ε^*	(R_x, R_y)	(xz, yz)
	1	ε^*	$-\varepsilon$	−1	$-\varepsilon^*$	ε	1	ε^*	$-\varepsilon$	−1	$-\varepsilon^*$	ε		
E_{2g}	1	$-\varepsilon^*$	$-\varepsilon$	1	$-\varepsilon^*$	$-\varepsilon$	1	$-\varepsilon^*$	$-\varepsilon$	1	$-\varepsilon^*$	$-\varepsilon$		(x^2-y^2, xy)
	1	$-\varepsilon$	$-\varepsilon^*$	1	$-\varepsilon$	$-\varepsilon^*$	1	$-\varepsilon$	$-\varepsilon^*$	1	$-\varepsilon$	$-\varepsilon^*$		
A_u	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	z	
B_u	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1		
E_{1u}	1	ε	$-\varepsilon^*$	−1	$-\varepsilon$	ε^*	−1	$-\varepsilon$	ε^*	1	ε	$-\varepsilon^*$	(x, y)	
	1	ε^*	$-\varepsilon$	−1	$-\varepsilon^*$	ε	−1	$-\varepsilon^*$	ε	1	ε^*	$-\varepsilon$		
E_{2u}	1	$-\varepsilon^*$	$-\varepsilon$	1	$-\varepsilon^*$	$-\varepsilon$	−1	ε^*	ε	−1	ε^*	ε		
	1	$-\varepsilon$	$-\varepsilon^*$	1	$-\varepsilon$	$-\varepsilon^*$	−1	ε	ε^*	−1	ε	ε^*		

.../13-

D_{6h}	E	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$	i	$2S_3$	$2S_6$	σ_h	$3\sigma_d$	$3\sigma_v$	(x axis coincident with C_2')	
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1		x^2+y^2, z^2
A_{2g}	1	1	1	1	−1	−1	1	1	1	1	−1	−1	R_z	
B_{1g}	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1		
B_{2g}	1	−1	1	−1	−1	1	1	−1	1	−1	−1	1		
E_{1g}	2	1	−1	−2	0	0	2	1	−1	−2	0	0	(R_x, R_y)	(xz, yz)
E_{2g}	2	−1	−1	2	0	0	2	−1	−1	2	0	0		(x^2-y, xy)
A_{1u}	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1		
A_{2u}	1	1	1	1	−1	−1	−1	−1	−1	−1	1	1	z	
B_{1u}	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1		
B_{2u}	1	−1	1	−1	−1	1	−1	1	−1	1	1	−1		
E_{1u}	2	1	−1	−2	0	0	−2	−1	1	2	0	0	(x, y)	
E_{2u}	2	−1	−1	2	0	0	−2	1	1	−2	0	0		

D_{4h}	E	$2C_4$	$2C_4^2$	$2C_4$	C_2	$4C_2'$	$4C_2''$	i	$2S_4^3$	$2S_4$	$2S_4$	σ_h	$4\sigma_v$	$4\sigma_d$	(x axis coincident with C_2')	
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1	1	1		x^2+y^2, z^2
A_{2g}	1	1	1	1	1	−1	−1	1	1	1	1	1	−1	−1	R_z	
B_{1g}	1	−1	−1	1	1	1	−1	1	−1	−1	1	1	1	−1		
B_{2g}	1	−1	−1	1	1	−1	1	1	−1	−1	1	1	−1	1		
E_{1g}	2	$\sqrt{2}$	$-\sqrt{2}$	0	−2	0	0	2	$\sqrt{2}$	$-\sqrt{2}$	0	−2	0	0	(R_x, R_y)	(xz, yz)
E_{2g}	2	0	0	−2	2	0	0	2	0	0	−2	2	0	0		(x^2-y^2, xy)
E_{3g}	2	$-\sqrt{2}$	$\sqrt{2}$	0	−2	0	0	2	$-\sqrt{2}$	$\sqrt{2}$	0	−2	0	0		
A_{1u}	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1		
A_{2u}	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	1	1	z	
B_{1u}	1	−1	−1	1	1	1	−1	−1	1	1	−1	−1	−1	1		
B_{2u}	1	−1	−1	1	1	−1	1	−1	1	1	−1	−1	1	−1		
E_{1u}	2	$\sqrt{2}$	$-\sqrt{2}$	0	−2	0	0	−2	$-\sqrt{2}$	$\sqrt{2}$	0	2	0	0	(x, y)	
E_{2u}	2	0	0	−2	2	0	0	−2	0	0	2	−2	0	0		
E_{3u}	2	$-\sqrt{2}$	$\sqrt{2}$	0	−2	0	0	−2	$\sqrt{2}$	$-\sqrt{2}$	0	2	0	0		

► *The D_{nd} Groups*

D_{2d}	E	$2S_4$	C_2	$2C_2'$	$2\sigma_d$	(x axis coincident with C_2')	
A_1	1	1	1	1	1		x^2+y^2, z^2
A_2	1	1	1	−1	−1	R_z	
B_1	1	−1	1	1	−1		x^2-y^2
B_2	1	−1	1	−1	1	z	xy
E	2	0	−2	0	0	$(x, y), (R_x, R_y)$	(xz, yz)

D_{3d}	E	$2C_3$	$3C_2$	i	$2S_6$	$3\sigma_d$	(x axis coincident with C_2)	
A_{1g}	1	1	1	1	1	1		x^2+y^2, z^2
A_{2g}	1	1	−1	1	1	−1	R_z	
E_g	2	−1	0	2	−1	0	(R_x, R_y)	$(x^2-y^2, xy); (xz, yz)$
A_{1u}	1	1	1	−1	−1	−1		
A_{2u}	1	1	−1	−1	−1	1	z	
E_u	2	−1	0	−2	1	0	(x, y)	

▸ *The D_{nh} Groups*

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$		
A_g	1	1	1	1	1	1	1	1		x^2, y^2, z^2
B_{1g}	1	1	−1	−1	1	1	−1	−1	R_z	xy
B_{2g}	1	−1	1	−1	1	−1	1	−1	R_y	xz
B_{3g}	1	−1	−1	1	1	−1	−1	1	R_x	yz
A_u	1	1	1	1	−1	−1	−1	−1		
B_{1u}	1	1	−1	−1	−1	−1	1	1	z	
B_{2u}	1	−1	1	−1	−1	1	−1	1	y	
B_{3u}	1	−1	−1	1	−1	1	1	−1	x	

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$	(x axis coincident with C_2)	
A_1'	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	−1	1	1	−1	R_z	
E'	2	−1	0	2	−1	0	(x, y)	$(x^2 - y^2, xy)$
A_1''	1	1	1	−1	−1	−1		
A_2''	1	1	−1	−1	−1	1	z	
E''	2	−1	0	−2	1	0	(R_x, R_y)	(xz, yz)

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$	(x axis coincident with C_2')	
A_{1g}	1	1	1	1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_{2g}	1	1	1	−1	−1	1	1	1	−1	−1	R_z	
B_{1g}	1	−1	1	1	−1	1	−1	1	1	−1		$x^2 - y^2$
B_{2g}	1	−1	1	−1	1	1	−1	1	−1	1		xy
E_g	2	0	−2	0	0	2	0	−2	0	0	(R_x, R_y)	(xz, yz)
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1		
A_{2u}	1	1	1	−1	−1	−1	−1	−1	1	1	z	
B_{1u}	1	−1	1	1	−1	−1	1	−1	−1	1		
B_{2u}	1	−1	1	−1	1	−1	1	−1	1	−1		
E_u	2	0	−2	0	0	−2	0	2	0	0	(x, y)	

D_{5h}	E	$2C_5$	$2C_5^2$	$5C_2$	σ_h	$2S_5$	$2S_5^3$	$5\sigma_v$	(x axis coincident with C_2)	
A_1'	1	1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	1	−1	1	1	1	−1	R_z	
E_1'	2	2 cos 72°	2 cos 144°	0	2	2 cos 72°	2 cos 144°	0	(x, y)	
E_2'	2	2 cos 144°	2 cos 72°	0	2	−2 cos 144°	2 cos 72°	0		$(x^2 - y^2, xy)$
A_1''	1	1	1	1	−1	−1	−1	−1		
A_2''	1	1	1	−1	−1	−1	−1	1	z	
E_1''	2	2 cos 72°	2 cos 144°	0	−2	−2 cos 72°	−2 cos 144°	0	(R_x, R_y)	(xz, yz)
E_2''	2	2 cos 144°	2 cos 72°	0	−2	−2 cos 144°	−2 cos 72°	0		

T_h	E	$4C_3$	$4C_3^2$	$3C_2$	i	$4S_6$	$4S_6^5$	$3\sigma_h$	($\varepsilon = \exp(2\pi i/3)$	
A_g	1	1	1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_u	1	1	1	1	−1	−1	−1	−1		
E_g	1	ε	ε^*	1	1	ε	ε^*	1		$(2z^2 - x^2 - y^2,$ $x^2 - y^2)$
	1	ε^*	ε	1	1	ε^*	ε	1		
E_u	1	ε	ε^*	1	−1	$-\varepsilon$	$-\varepsilon^*$	−1		
	1	ε^*	ε	1	−1	$-\varepsilon^*$	$-\varepsilon$	−1		
T_g	3	0	0	−1	3	0	0	−1	(R_x, R_y, R_z)	(xz, yz, xy)
T_u	3	0	0	−1	−3	0	0	1	(x, y, z)	

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$		
A_1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_2	1	1	1	−1	−1		$(2z^2 - x^2 - y^2, x^2 - y^2)$
E	2	−1	2	0	0		
T_1	3	0	−1	1	−1	(R_x, R_y, R_z)	(xy, xz, yz)
T_2	3	0	−1	−1	1	(x, y, z)	

▸ *Octahedral Groups*

O	E	$6C_4$	$3C_2(=C_4^2)$	$8C_3$	$6C_2$		
A_1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_2	1	−1	1	1	−1		$(2z^2 - x^2 - y^2, x^2 - y^2)$
E	2	0	2	−1	0		
T_1	3	1	−1	0	−1	$(R_x, R_y, R_z), (x, y, z)$	(xy, xz, yz)
T_2	3	−1	−1	0	1		

O_h	E	$8C_3$	$6C_2$	$6C_4$	$3C_2(=C_4^2)$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_{2g}	1	1	−1	−1	1	1	−1	1	1	−1		$(2z^2 - x^2 - y^2, x^2 - y^2)$
E_g	2	−1	0	0	2	2	0	−1	2	0		
T_{1g}	3	0	−1	1	−1	3	1	0	−1	−1	(R_x, R_y, R_z)	(xz, yz, xy)
T_{2g}	3	0	1	−1	−1	3	−1	0	−1	1		
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1		
A_{2u}	1	1	−1	−1	1	−1	1	−1	−1	1		
E_u	2	−1	0	0	2	−2	0	1	−2	0		
T_{1u}	3	0	−1	1	−1	−3	−1	0	1	1	(x, y, z)	
T_{2u}	3	0	1	−1	−1	−3	1	0	1	−1		

D_{4d}	E	$2S_8$	$2C_4$	$2S_8^3$	C_2	$4C_2'$	$4\sigma_d$	(x axis coincident with C_2')	
A_1	1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2	1	1	1	1	1	−1	−1	R_z	
B_1	1	−1	1	−1	1	1	−1		
B_2	1	−1	1	−1	1	−1	1	z	
E_1	2	$\sqrt{2}$	0	$-\sqrt{2}$	−2	0	0	(x, y)	
E_2	2	0	−2	0	2	0	0		$(x^2 - y^2, xy)$
E_3	2	$-\sqrt{2}$	0	$\sqrt{2}$	−2	0	0	(R_x, R_y)	(xz, yz)

D_{5d}	1	$2C_5$	$2C_5^2$	$5C_2$	i	$2S_{10}^3$	$2S_{10}$	$5\sigma_d$	(x axis coincident with C_2)	
A_{1g}	1	1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_{2g}	1	1	1	−1	1	1	1	−1	R_z	
E_{1g}	2	2 cos 72°	2 cos 144°	0	2	2 cos 72°	2 cos 144°	0	(R_x, R_y)	(xz, yz)
E_{2g}	2	2 cos 144°	2 cos 72°	0	2	2 cos 144°	2 cos 72°	0		$(x^2 - y^2, xy)$
A_{1u}	1	1	1	1	−1	−1	−1	−1		
A_{2u}	1	1	1	−1	−1	−1	−1	1	z	
E_{1u}	2	2 cos 72°	2 cos 144°	0	−2	−2 cos 72°	−2 cos 144°	0	(x, y)	
E_{2u}	2	2 cos 144°	2 cos 72°	0	−2	−2 cos 144°	−2 cos 72°	0		

D_{6d}	E	$2S_{12}$	$2C_6$	$2S_4$	$2C_3$	$2S_{12}^5$	C_2	$6C_2'$	$6\sigma_d$	(x axis coincident with C_2)	
A_1	1	1	1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2	1	1	1	1	1	1	1	−1	−1	R_z	
B_1	1	−1	1	−1	1	−1	1	1	−1		
B_2	1	−1	1	−1	1	−1	1	−1	1	z	
E_1	2	$\sqrt{3}$	1	0	−1	$-\sqrt{3}$	−2	0	0	(x, y)	
E_2	2	1	−1	−2	−1	1	2	0	0		$(x^2 - y^2, xy)$
E_3	2	0	−2	0	2	0	−2	0	0		
E_4	2	−1	−1	2	−1	−1	2	0	0		
E_5	2	$-\sqrt{3}$	1	0	−1	$\sqrt{3}$	−2	0	0	(R_x, R_y)	(xz, yz)

THE CUBIC GROUPS

▸ *Tetrahedral Groups*

T	E	$4C_3$	$4C_3^2$	$3C_2$	$\varepsilon = \exp(2\pi i/3)$	
A	1	1	1	1		$x^2 + y^2 + z^2$
E	$\begin{Bmatrix} 1 & \varepsilon & \varepsilon^* & 1 \\ 1 & \varepsilon^* & \varepsilon & 1 \end{Bmatrix}$					$(2z^2 - x^2 - y^2, x^2 - y^2)$
T	3	0	0	−1	$(R, R_y, R_z), (x, y, z)$	(xy, xz, yz)

[KTE 211]

LAMPIRAN

Pemalar Asas dalam Kimia Fizik

Simbol	Keterangan	Nilai
N_A	Nombor Avogadro	6.022×10^{23} mol^{-1}
F	Pemalar Faraday	96,500 C mol^{-1}, atau coulomb per mol, elektron
e	Cas elektron	4.80×10^{-10} esu 1.60×10^{-19} C atau coulomb
m_e	Jisim elektron	9.11×10^{-28} g 9.11×10^{-31} kg
m_p	Jisim proton	1.67×10^{-24} g 1.67×10^{-27} kg
h	Pemalar Planck	6.626×10^{-27} erg s 6.626×10^{-34} J s
c	Halaju cahaya	3.0×10^{10} cm s^{-1} 3.0×10^{8}m s^{-1}
R	Pemalar gas	8.314×10^{7} erg K^{-1} mol^{-1} 8.314 J K^{-1} mol^{-1} 0.082 *l* atm K^{-1} mol^{-1} 1.987 cal K^{-1} mol^{-1}
k	Pemalar Boltzmann	1.380×10^{-16} erg K^{-1} molekul^{-1} 1.380×10^{-23} J K^{-1} molekul^{-1}
g		981 cm s^{-2} 9.81 m s^{-2}
1 atm		76 cmHg 1.013×10^{6} dyne cm^{-2} 101,325 N m^{-2}
$2.303 \frac{RT}{F}$		0.0591 V, atau volt, pada 25 °C

Berat Atom yang Berguna

H = 1.0	C = 12.0	I = 126.9	Fe = 55.8	As = 74.9
Br = 79.9	Cl = 35.5	Ag = 107.9	Pb = 207.0	Xe = 131.1
Na = 23.0	K = 39.1	N = 14.0	Cu = 63.5	F = 19.0
O = 16.0	S = 32.0	P = 31.0	Ca = 40.1	Mg = 24.0
Sn = 118.7	Cs = 132.9	Te = 128.0		